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Kalakul, Sawitree; Kontogeorgis, Georgios; Gani, Rafiqul

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Sawitree Kalakul, Georgios M. Kontogeorgis, Rafiqul Gani

The Virtual Product-Process Design Laboratory (VPPD-Lab) has been developed as a computer aided tool for product-process development. Rather than design chemicals based products through an experimental-based trial and error approach, the powerful methodologies and tools in VPPD-Lab help to replace some of experimental steps by performing virtual experiments using model-based approaches. VPPD-Lab offers a quick search of active ingredients, solvents, and additives that match the desired specification and to be followed by experimental-based validation, and evaluation of the most promising candidates for eventual selection of the final product reducing valuable time and resources at the primary design stage.

The previous version of VPPD-Lab consists of templates for the design of microcapsules, solvent selection, and homogeneous liquid formulated products such as paint formulation, sunscreen lotion, and insect repellent lotion [1]. The algorithms in VPPD-Lab can perform ingredients selection and testing, solubility tests, and property measurements using its available property models and chemical databases. VPPD-Lab also can directly access to ICAS (Integrated Computer Aided System) [2] as a support tool to (i) consult several chemical databases using ICAS database manager, (ii) predict property values which are missing in the databases predicted through the ICAS property prediction tool (ProPred), and (iii) perform process design using process models available in ICAS MOT (Modeling testbed) to design the processes. Therefore, VPPD-Lab is a complete software for product-process design. However, the main limitations of property models available in the software should be extended in order to enlarge the application range of the models, and able to apply to a wider range of problems. Such approaches require the use and management of a wide range of property models, calculation procedures and a very large amount of data. A systematic framework to manage the data and models are necessary as well as the modules for a better communication between VPPD-Lab and support tools.

This work proposes a systematic framework to improve and extend the application range of VPPD-Lab. Various property prediction models have been developed and integrated to the different steps of the design algorithms. The chemical databases, and property models needed for each type of products are managed through a knowledge base representation system enabling a flexible and efficient communication between the templates and supporting tools (databases, models, and connected software). The new version of VPPD-Lab has included new templates of the design of blended and emulsified products [3,4] with the new user interface of a generic workflow to design products and processes. Therefore, VPPD-Lab is now generic, user friendly, and widely applicable with options for a wide range of chemicals based liquid products.

A case study dealing with tailor-made design of jet-fuels is highlighted to illustrate the application of the developed methods for blended liquid formulation implemented in VPPD-Lab.

References

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